Variable Density Effects in Stochastic Lagrangian Models for Turbulent Combustion

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1 Introduction

PDF methods have proven useful in modelling turbulent combustion, primarily be-
cause convection and complex reactions can be treated without the need for turbulence-
modelling approximations. Xu & Pope [14,16] and Tang et al. [17] provide recent ex-
amples of such model calculations based on the modelled transport equation for the
joint PDF of velocity, turbulent frequency and composition (species mass fractions
and enthalpy).

The advantages of PDF methods in dealing with chemical reaction and convec-
tion are preserved irrespective of density variation. Since the density variation in a
typical combustion process may be as large as a factor of seven, including variable-
density effects in PDF methods is of significance. Conventionally, the strategy of
modelling variable density flows in PDF methods is similar to that used for second-
moment closure models (SMCM): models are developed based on a constant-density
formulation, and then the same models are used for variable-density flows, but with
density-weighted statistics in place of Reynolds averages. However, it is not clear
to what extent this strategy is legitimate. First, the coefficients in these models are
deduced from experimental data or simple turbulent shear flows of constant density;
second, the impact of density variation on the model formulation is not considered.
However, taking account of density variation in turbulence models is not an easy
task due to the lack of good experimental and theoretical understanding of density
variation effects.

Second-moment closure models for variable-density flows have been advanced by
a number of researches [1,3,4,9,11]. Recently, Lindstedt and Váos (1999) [6] im-
proved the pressure-strain-rate term, specifically the isotropization of production
model (IPM), by considering the preferential acceleration effect.

There is a close relationship between PDF models and second moment closure
models which has previously been exploited to improve the modelling in both ap-
proaches [2,8,13,18]. In this paper we develop a PDF model, incorporating variable-
density effects, which is consistent with the SMCM of Lindstedt & Váos [6]. We first
consider the Reynolds stress model and deduce a consistent PDF model for velocity;
we then deduce a consistent model for the turbulence frequency.

2 Second Moment Closure Equations

With few exceptions (e.g., [9]), moment closure models solve transport equations for
density-weighted quantities. The decomposition as used in [4] is

$$U_i = \widetilde{U}_i + u_i'', \quad \xi = \widetilde{\xi} + \xi'', \tag{1}$$

$$\rho = \langle\rho\rangle + \rho', \quad p = \langle p\rangle + p',$$

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where $\mathbf{U}, \rho, p$ and ξ represent the fluid velocity, density, pressure and a scalar variable (e.g., mixture fraction in nonpremixed flames), respectively; and $\tilde{}$ and $\langle\,\rangle$ denote density-weighted (Favre) means, and volume-weighted (Reynolds) means, respectively.

2.1 Exact Reynolds Stress Equation

To simplify the notation, we use R_{ij} to denote the density-weighted Reynolds stress:

$$R_{ij} \equiv \widetilde{u_i'' u_j''} = \langle \rho u_i'' u_j'' \rangle / \langle \rho \rangle. \tag{2}$$

The exact Reynolds-stress equation for variable density flow can be written [4,6]:

$$\langle \rho \rangle \frac{\overline{D} R_{ij}}{\overline{D} t} + \frac{\partial}{\partial x_\ell} T_{ij\ell} = \langle \rho \rangle P_{ij} + \Phi_{ij} + \phi_{ij} - \langle \rho \rangle \varepsilon_{ij}, \tag{3}$$

where

$$\frac{\overline{D}}{\overline{D} t} \equiv \frac{\partial}{\partial t} + \tilde{U}_\ell \frac{\partial}{\partial x_\ell}, \tag{4}$$

is the mean convective derivative;

$$T_{ij\ell} \equiv \langle \rho u_i'' u_j'' u_\ell'' \rangle / \langle \rho \rangle, \tag{5}$$

is the triple correlation;

$$P_{ij} \equiv -R_{i\ell} \frac{\partial \tilde{U}_j}{\partial x_\ell} - R_{j\ell} \frac{\partial \tilde{U}_i}{\partial x_\ell}, \tag{6}$$

is the production;

$$\Phi_{ij} \equiv -\langle u_i'' \rangle \frac{\partial \langle p \rangle}{\partial x_j} - \langle u_j'' \rangle \frac{\partial \langle p \rangle}{\partial x_i}, \tag{7}$$

is the mean pressure gradient term;

$$\phi_{ij} \equiv -\left\langle u_i'' \frac{\partial p'}{\partial x_j} + u_j'' \frac{\partial p'}{\partial x_i} \right\rangle, \tag{8}$$

is the fluctuating pressure gradient term; and $\langle \rho \rangle \varepsilon_{ij}$ is the viscous dissipation tensor. The fluctuating pressure gradient term is decomposed as [6]

$$\phi_{ij} = \phi_{ij}^R + \phi_{ij}^D + \phi_{ij}^T, \tag{9}$$

where

$$\phi_{ij}^R \equiv \phi_{ij} - \frac{1}{3} \phi_{\ell\ell} \delta_{ij}, \tag{10}$$

$$\phi_{ij}^D \equiv \frac{2}{3} \delta_{ij} \left\langle p' \frac{\partial u_\ell''}{\partial x_\ell} \right\rangle, \tag{11}$$

and

$$\phi_{ij}^T \equiv -\frac{2}{3} \delta_{ij} \frac{\partial}{\partial x_\ell} \langle p' u_\ell'' \rangle. \tag{12}$$

It may be observed that in constant-density flow Φ_{ij} and ϕ_{ij}^D are zero.

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2.2 Modelled Reynolds Stress Equation

The modelling focuses on the term ϕ_{ij}^R. Lindstedt & Váos discuss the terms ϕ_{ij}^D and ϕ_{ij}^T, but in the end either neglect them or absorb them into other modelled terms. Their model can then be written

$$\phi_{ij} - \langle\rho\rangle\varepsilon_{ij} = \langle\rho\rangle(G_{i\ell}R_{\ell j} + G_{j\ell}R_{\ell i} + C_0\varepsilon\delta_{ij})$$
$$+ C_{A_R}(\Phi_{ij} - \frac{2}{3}\Phi\delta_{ij}), \tag{13}$$

where the tensor G_{ij} and the constant $C_0 = 2.1$ arise from the generalized Langevin model [2]; $\varepsilon = \frac{1}{2}\varepsilon_{ii}$ is the dissipation; $C_{A_R} = -3/10$; and

$$\Phi \equiv \frac{1}{2}\Phi_{ii} = -\langle u_i''\rangle\frac{\partial\langle p\rangle}{\partial x_i}. \tag{14}$$

The terms in G_{ij} and C_0 represent the constant-density model, whereas the term in Φ_{ij} is the addition to account for variable-density effects.

For future reference we write the (partially) modelled Reynolds stress equation obtained by substituting Eq.(13) into Eq.(3). The result is

$$\langle\rho\rangle\frac{\overline{D}R_{ij}}{\overline{D}t} + \frac{\partial T_{ij\ell}}{\partial x_\ell} = \langle\rho\rangle P_{ij} + \Phi_{ij}$$
$$+ \langle\rho\rangle(G_{i\ell}R_{\ell j} + G_{j\ell}R_{\ell i} + C_0\varepsilon\delta_{ij})$$
$$+ C_{A_R}\left(\Phi_{ij} - \frac{2}{3}\Phi\delta_{ij}\right). \tag{15}$$

2.3 Model Equations for k, ε and ω

The exact equation for the Favre mean turbulent kinetic energy

$$k \equiv \frac{1}{2}R_{ii} = \frac{1}{2}\widetilde{u_i''u_i''}, \tag{16}$$

is obtained by taking half the trace of Eq.(3). Neglecting the term $\frac{1}{2}\phi_{ii}$, the result is:

$$\langle\rho\rangle\frac{\overline{D}k}{\overline{D}t} + \frac{\partial}{\partial x_\ell}\left(\frac{1}{2}T_{ii\ell}\right) = \langle\rho\rangle(P - \varepsilon) + \Phi. \tag{17}$$

The GLM coefficient G_{ij} satisfy the constraint

$$G_{ij}R_{ij} + \left(1 + \frac{3}{2}C_0\right)\varepsilon = 0, \tag{18}$$

so that half the trace of the modelled Reynolds-stress equation is identical to Eq.(17).

The standard model equation for the Favre mean dissipation [4] is

$$\langle\rho\rangle\frac{\overline{D}\varepsilon}{\overline{D}t} + \mathcal{T}_\varepsilon = \langle\rho\rangle\frac{\varepsilon}{k}(C_{\varepsilon1}P - C_{\varepsilon2}\varepsilon) + C_{\varepsilon3}\frac{\varepsilon}{k}\Phi, \tag{19}$$

where $\mathcal{T}_\varepsilon$ is a transport term, and the values of the constants given by Lindstedt & Váos [6] are $C_{\varepsilon1} = 1.44, C_{\varepsilon2} = 1.92$ and $C_{\varepsilon3} = 1.2$. The term in $C_{\varepsilon3}$ is of course zero in constant-density flow.

We also consider the model equation for the Favre mean turbulence frequency $\tilde{\omega} \equiv \varepsilon/k$ that follows from the above equations:

$$\begin{aligned}
\langle\rho\rangle\frac{\overline{D}\tilde{\omega}}{\overline{D}t} &= \frac{\langle\rho\rangle}{k}\frac{\overline{D}\varepsilon}{\overline{D}t} - \frac{\langle\rho\rangle\varepsilon}{k^2}\frac{\overline{D}k}{\overline{D}t} \\
&= \mathcal{T}_\omega + \langle\rho\rangle\tilde{\omega}^2\left(C_{\omega2} - C_{\omega1}\frac{P}{\varepsilon}\right) + C_{\omega3}\frac{\tilde{\omega}\Phi}{k},
\end{aligned} \tag{20}$$

where $\mathcal{T}_\omega$ arises from the transport terms in the k and ε equations, and $C_{\omega\alpha} = C_{\varepsilon\alpha} - 1$, for $\alpha = 1, 2, 3$, i.e.,

$$C_{\omega1} = 0.44, \quad C_{\omega2} = 0.92, \quad C_{\omega3} = 0.2.$$

3 PDF Model Equations

As usual [7,19], we approach PDF modelling from the Lagrangian viewpoint by considering stochastic models for the position $\mathbf{X}^*(t)$, velocity $\mathbf{U}^*(t)$, turbulence frequency $\omega^*(t)$ and composition $\xi^*(t)$ of a fluid particle. The models proposed here are:

$$dX_i^*(t) = U_i^*(t)\,dt, \tag{21}$$

$$\begin{aligned}
dU_i^* &= -\left(\frac{C_a}{\rho^*} + \frac{1 - C_a}{\langle\rho\rangle}\right)\frac{\partial\langle p\rangle}{\partial x_i}\,dt \\
&\quad + (G_{ij} + G_{ij}^A)(U_j^* - \tilde{U}_j)\,dt + (C_0\varepsilon + E)^{\frac{1}{2}}dW_i,
\end{aligned} \tag{22}$$

and

$$d\omega^*(t) = -C_3(\omega^* - \tilde{\omega})\Omega dt - S_\omega\Omega\omega^*(t)dt + [2C_3C_4\tilde{\omega}\Omega\omega^*]^{\frac{1}{2}}\,dW. \tag{23}$$

The quantities appearing in these equations are defined below as each equation is discussed in turn. (A specific model for $\xi^*(t)$ is not needed in the subsequent development.)

3.1 Velocity Model

In the velocity equation, G_{ij} and C_0 are the same GLM coefficients as appear in the Reynolds stress model, and $\mathbf{W}(t)$ is an isotropic Wiener process. For simplicity, we do not consider here a model for the pressure transport [15].

The coefficient C_a, E and G_{ij}^A are to be determined: if they are set to zero, then Eq.(22) corresponds to the usual constant-density GLM, *which corresponds to Eq.(15)* at the Reynolds stress level (for constant-density flow).

The coefficient C_a is particularly significant, since it determines how the mean pressure gradient accelerates fluid of different density. (ρ^* denotes the density of the particle.) For $C_a = 0$, the term corresponds

$$\frac{D\mathbf{U}}{Dt} = -\frac{1}{\langle\rho\rangle}\nabla\langle p\rangle,$$
(24)

implying that all fluid elements experience the same acceleration, independent of their density. Conversely, for $C_a = 1$, the term corresponds to

$$\frac{D\mathbf{U}}{Dt} = -\frac{1}{\rho}\nabla\langle p\rangle,$$
(25)

implying that the pressure force per unit volume experienced by the fluid is independent of its density, and hence less dense fluid is preferentially accelerated. At first glance, the exact Navier-Stokes equations suggest that Eq.(25) is the appropriate model—but this ignores the phenomenon of "added mass." As the less dense fluid accelerates, so also does the more dense fluid that it displaces. Hence, we expect the appropriate value of C_a to be between 0 and 1.

From the stochastic model for $\mathbf{U}^*(t)$ (Eq.(22)), standard techniques [7,8] can be used to derive the corresponding model equations for the mean velocity $\tilde{\mathbf{U}}$ and for the Reynolds stresses R_{ij}. The mean momentum equation is

$$\langle\rho\rangle\frac{\overline{D}\tilde{U}_i}{\overline{D}t} = -\frac{\partial}{\partial x_j}(\langle\rho\rangle R_{ij}) - \frac{\partial\langle p\rangle}{\partial x_i}.$$
(26)

This equation is free of model coefficients, and (apart from the neglect of the viscous term) it is the exact Reynolds equation stemming from the Navier-Stokes equation.

The Reynolds stress equation derived from Eq.(22) is :

$$\langle\rho\rangle\frac{\overline{D}R_{ij}}{\overline{D}t} + \frac{\partial}{\partial x_\ell}T_{ij\ell} = \langle\rho\rangle P_{ij} + C_a\Phi_{ij}$$
$$+\langle\rho\rangle[(G_{i\ell} + G_{i\ell}^A)R_{\ell j} + (G_{j\ell} + G_{j\ell}^A)R_{\ell i} + (C_0\varepsilon + E)\delta_{ij}].$$
(27)

By comparing this equation to the model of Lindstedt & Váos (Eq.(15)), we see that these two equations are identical if the coefficients C_a, G_{ij}^A and E are chosen to satisfy the constraint:

$$\Phi_{ij} + C_{A_R}\left(\Phi_{ij} - \frac{2}{3}\Phi\delta_{ij}\right) = C_a\Phi_{ij} + \langle\rho\rangle(E\delta_{ij} + G_{i\ell}^A R_{\ell j} + G_{j\ell}^A R_{\ell i}).$$
(28)

Clearly, based on consistency with Lindstedt & Váos' model, the appropriate choice of C_a is

$$C_a = 1 + C_{A_R} = \frac{7}{10}.$$ (29)

Then the consistency condition reduces to

$$\frac{2}{3}(1 - C_a)\Phi\delta_{ij} = \langle\rho\rangle(E\delta_{ij} + G_{i\ell}^A R_{\ell j} + G_{j\ell}^A R_{\ell i}).$$ (30)

We now consider three ways to satisfy Eq.(30) exactly or approximately. The simplest specification of E and G_{ij}^A to satisfy Eq.(30) is

$$E = \frac{2}{3}(1 - C_a)\Phi/\langle\rho\rangle, \quad G_{ij}^A = 0.$$ (31)

This is not, however, an acceptable model since it does not guarantee that the stochastic model for $\mathbf{U}^*(t)$ (Eq.(22)) is realizable. To be realizable, the coefficient $C_0\varepsilon + E$ must be non-negative, which is not assured by Eq.(31).

The second specification of G_{ij}^A and E considered is

$$E = 0, \quad G_{ij}^A = \frac{(1 - C_a)\Phi}{3\langle\rho\rangle} R_{ij}^{-1},$$ (32)

where R_{ij}^{-1} denotes the inverse of the Reynolds-stress tensor (such that $R_{ij}^{-1} R_{jk} = \delta_{ik}$). As may be directly verified by substitution, this specification exactly satisfies the constraint equation, Eq.(30).

To avoid the complexity involved in the inverse R_{ij}^{-1}, we consider the third specification

$$E = 0, \quad G_{ij}^A = \frac{(1 - C_a)\Phi}{2\langle\rho\rangle k}\delta_{ij}.$$ (33)

This does not satisfy the constraint equation, Eq.(30), but it does satisfy its trace. Consequently, compared to Lindstedt & Váos' model, Eq.(33) leads to the additional term in the Reynolds-stress equation

$$\frac{\overline{D}R_{ij}}{\overline{D}t} = \ldots (1 - C_a)\Phi\left(R_{ij}/k - \frac{2}{3}\delta_{ij}\right).$$ (34)

The occurrence of k in the denominator of Eq.(33), and similarly R_{ij}^{-1} in Eq.(32), raises questions of realizability as k tends to zero. However, when used in the stochastic model for $\mathbf{U}^*(t)$, both specifications are realizable. Using Eq.(32), for example, the relevant coefficient in the stochastic model (Eq.(22)) is

$$G_{ij}^A(U_j^* - \tilde{U}_j) = \frac{(1 - C_a)\Phi}{3\langle\rho\rangle} R_{ij}^{-1}(U_j^* - \tilde{U}_j)$$

$$= -\frac{(1 - C_a)}{3\langle\rho\rangle}\frac{\partial\langle p\rangle}{\partial x_i}\left\{\frac{\langle u_i''\rangle}{k^{\frac{1}{2}}}\right\}\left\{kR_{ij}^{-1}\right\}\left\{\frac{U_j^* - \tilde{U}_j}{k^{\frac{1}{2}}}\right\}.$$ (35)

Each term in braces is a non-dimensional quantity which is bounded as k tends to zero (or, more precisely, as the smallest Reynolds normal stress tends to zero).

To summarize the principal result: the stochastic model for velocity Eq.(22), with $C_a = 1 + C_{A_R} = 0.7, E = 0$ and G_{ij}^A given by Eq.(32) is realizable and corresponds at the Reynolds stress level to the model of Lindstedt & Váos.

3.2 Turbulent Frequency Model

The stochastic model for turbulent frequency (Eq.(23)) is that given by Van Slooten, Jayesh & Pope [12]. The quantities $\omega^*, \tilde{\omega}$ and Ω are, respectively, the particle frequency, the (Favre mean) particle frequency, and the condition-mean frequency which is designed to account for external intermittency and whose definition is given in [12]. For fully developed turbulence, Ω equals $\tilde{\omega}$, and in general the dissipation is given by $\varepsilon = k\Omega$. In the final term in Eq.(23), $W(t)$ is a Wiener process, independent of that in the velocity model. The values of the constants give in [12] are $C_3 = 1.0$ and $C_4 = 0.25$.

The equation for the mean turbulent frequency deduced from the stochastic model (Eq.(23)) is :

$$\langle \rho \rangle \frac{\overline{D\tilde{\omega}}}{\overline{Dt}} = -\frac{\partial}{\partial x_i}[\langle \rho \rangle \widetilde{u_i''\omega}] - S_\omega \Omega \tilde{\omega}. \tag{36}$$

If Ω and $\tilde{\omega}$ are assumed to be equal (as they are in homogeneous turbulence), then the source term in this equation is consistent with that in the standard model (Eq.(20)), if S_ω is taken to be

$$S_\omega = C_{\omega 1}\frac{P}{\varepsilon} - C_{\omega 2} - C_{\omega 3}\frac{\Phi}{k\Omega}. \tag{37}$$

The first two terms correspond to the standard constant-density model [12]. Hence, the conclusion is that the stochastic model for ω^* is consistent with Lindstedt and Váos' model, if the term in $C_{\omega 3}$ is included in the specification of S_ω.

The occurence of k in the denominator of Eq.(37) again raises concerns about realizability. An analysis of the k and $\tilde{\omega}$ equations shows that the model is realizable, but that it can cause k and ε to become zero in finite time. Because this is difficult to handle in numerical implementations, it is preferable to replace $\Phi/(k\Omega)$ in Eq.(37) by the well-conditioned approximation

$$\hat{\Phi} \equiv \frac{\Phi}{k\Omega + \gamma|\Phi|}, \tag{38}$$

where γ is a small positive constant (e.g., $\gamma = 0.1$).

3.3 Scalar Flux Equation

Given a stochastic model $\xi^*(t)$ for a scalar ξ, a modelled equation for the scalar flux $\widetilde{u_i''\xi''}$ can be deduced from the models for ξ^* and $\mathbf{U}^*$ [8].

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The full scalar flux equation depends, of course, on the mixing model contained in the model $\xi^*(t)$. But we note here just the terms arising from variable-density modifications to the velocity equation. With G_{ij}^A and E given by Eq.(32), these contributions are:

$$\langle\rho\rangle\frac{\overline{D}}{\overline{Dt}}\widetilde{u_i''\xi''} = \ldots - \frac{\partial\langle p\rangle}{\partial x_k}\left\{C_a\langle\xi''\rangle\delta_{ik} + \frac{1}{3}(1-C_a)R_{ij}^{-1}\langle u_k''\rangle\widetilde{u_j''\xi''}\right\}. \tag{39}$$

4 Conclusions

The variable-density turbulence model of Lindstedt & Váos [6] has been extended to the level of a PDF model. The resulting stochastic model for velocity (Eq.(22)) is an extension of the constant-density Generalized Langevin Model. The coefficients of the additional terms in this model equation are determined by requiring consistency with Lindstedt & Váos' model (Eq.(29) and Eq.(32)). The stochastic model for turbulence frequency is made consistent through the addition of a source term (Eq.(37)).

The model proposed here has yet to be implemented and evaluated in different circumstances by comparing its predictions to experimental data; and it is, of course, desirable that this be done. But nevertheless, the model's performance can be expected to be reasonable, in view of its close connection to Lindstedt & Váos' model — which has been evaluated.

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6 References

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